Activity of Withania somnifera against Herpes through deactivation of Herpes Simplex virus Type II Protease (1AT3)

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Abstract: An in-silico study was performed to determine the activity of Withania somnifera against Herpes. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Herpes Simplex virus Type II Protease (1AT3) enzyme. It was found that Rosmarinic acid helped to prevent Herpes.

Introduction: Withania somnifera is known for its medicinal activities. The medicinal plants are widely used by the traditional medical practitioners for curing various diseases like diarrhea, dysentery, insect bites, anemia, albuminuria, diabetes, herpes, etc.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophyta
Class	Magnoliopsida
Order	Solanales
Family	Solanaceae
Genus	Withania
Species	somnifera

Major phytochemicals present in the plant are:

- a. Sulforaphane
- b. Tannic acid
- c. Rosmarinic acid
- d. Cryptoxanthin

One of the major enzymes required for the survival of the organism causing Herpes is Herpes Simplex virus Type II Protease (1AT3) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

ISSN: 2395-6216